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Microscopic structural and dynamical properties of amorphous metallic alloy Ni33Zr67 at the temperature T=300K

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Abstract

We study the structural properties and the collective microscopic dynamics of atoms in the amorphous metallic alloy Ni33Zr67 at the temperature T=300K by molecular dynamics simulations. The calculated equilibrium structural and dynamical characteristics are compared with the experimental data on neutron diffraction and on inelastic X-ray scattering. We present the interpretation of observed structural relaxation of the microscopic density fluctuations of particles for amorphous metallic alloy in the framework of the recurrent relation approach. The results of theoretical calculations of the intensity of scattering I(k,ω) for amorphous Ni33Zr 67 are in a good agreement with the results of computer simulation as well as with the experimental data on inelastic X-ray scattering.

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